

# FILVERT SOFTWARE FOR COMPUTING FLUID FLUX VELOCITIES AND HEAT FLOW DENSITY FROM GEOTHERMAL DATA

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**Key Words:** deep heat flow density, fluid flux velocities, borehole thermal data, numerical treatment techniques

## ABSTRACT

A numerical algorithm FILVERT is proposed for processing borehole thermal data (temperature, heat conductivity, and heat production). The thermal data is used to study structure and kinematics of the fluid fluxes (vertical variations of the advection velocity  $v$ ) in the borehole section and to determine the deep heat flow density  $q_0$  at the drilling site (hydrogeological information need not be invoked).

## 1. INTRODUCTION

Borehole thermometric investigations are an important source of information about the thermal and fluid regime of the Earth's crust. The conductive heat flow density  $q_c$ , obtained from these measurements serves as a unique direct reflection of the energy effect of processes occurring in the interior. This parameter

$$q_c = -I \operatorname{grad} T, \quad (1)$$

where  $I$  is the thermal conductivity and  $T$  is the temperature, was estimated at about 30000 sites over the Earth's surface, including ocean and sea floors. However,  $q_c$  does not reflect the actual value of deep heat flow density at the measurement site because of many disturbing factors (see the review by Kononov and Polyak [1970]).

Among these factors, the movement of underground water is of particular interest. As early as 1956 N.A. Ogil'vi [1956] concluded that fluxes of underground water (at a velocity of a few mm per yr and greater) should control the heat transfer in the sedimentary cover, so that the remaining disturbances can be neglected. That is why borehole thermal data are considered as a sensitive indicator of the crustal hydrodynamics [e.g., Bredehoeft and Papadopoulos, 1965]. However, evaluating the fluid advection effect on the geothermal field presents severe difficulties. (Hereafter, according to the widely-distributed lexical standard, we consider the "advection" as a mass flux along the direct trajectory in contradistinction to the "convection", that is the flux along its cyclic trajectory). On the one hand, independent hydrogeological information used for this purpose [e.g., Lal'ko, 1974] is usually of a general character and, therefore, is not sufficient to reliably determine deep heat flow density  $q_0$  at specific sites of thermal measurements. On the other hand, evaluation of the fluid flux velocities by the graphic treatment of the borehole thermal data [Bredehoeft and Papadopoulos, 1965] is often of doubtful value because of significant variations of the thermal conductivity  $I$  with depth introducing large errors into the  $I$  averaging procedure. In parallel with  $I$ , the thermal gradient varies widely as usual, and

their product  $q_c$  varies considerably, as well. A dramatic increase of  $q_c$  with depth was found in many holes [Polyak and Smirnov, 1968; Sergienko, 1996, and others]. Its value below the measurement interval remains unclear and is sometimes estimated by a simple extrapolation. However, such an estimation is fairly subjective.

The purpose of this paper is to demonstrate the possibilities of the numerical algorithm FILVERT for computing the fluid flow velocity variations with depth on the basis of borehole thermal data, and of the related graphic-analytical procedure for estimating deep heat flow density.

## 2. TECHNIQUES FOR NUMERICAL TREATMENT OF THE THERMAL DATA

### 2.1 Quality of the original data

Various versions of the FILVERT software, beginning with the original [Yakovlev, 1985], were applied in processing the geothermal data from several holes drilled in the areas of the Caucasian Mineral'nye Vody, Transcaucasia (Saatly super deep hole), and the Pannonian basin (Szombathely-II hole). The original data used in the code are the temperature  $T(z)$ , heat conductivity  $I(z)$ , and heat production  $A(z)$ ; all these values are measured (determined) at different depths  $z$ .

Figure 1 shows the general view of the vertical distribution of the parameters  $T$ ,  $I$ , and their derivatives,  $\operatorname{grad} T$  and  $q_c$ , measured in holes at a depth of 2-2.5 km, examined by the proposed method. Naturally, only holes that have been standing for a long time after drilling are considered. The temperature distribution was examined in great detail, at depth steps from a few meters to 10-20 m, depending on the current geothermal gradient. Gradient values varied over a wide range, up to one order of magnitude. The variations in the heat conductivity are followed in lesser detail, and only a few locations in the given diagram are characterized by more than one point. The resultant heat flow density distribution only partly reflects the actual local values of its multipliers,  $I$  and  $\operatorname{grad} T$ , and is also essentially stochastic in nature.

The vertical variations in the heat production  $A$  are usually traced in much less detail than those of the first two parameters. However, this has almost no influence on the accuracy of the net result. The introduction of single measured or reference values of  $A$  changes the final solution by no more than a few percentage points.

Thus, the original thermal data are appreciably random in character. The proposed software takes this factor into account. Apart from these data, invoking additional geological information (depth position of lithological and hydrodynamic

discontinuities, etc.) greatly assists in obtaining a preliminary outline of the correct design depth intervals.

## 2.2 Mathematical description of the FILVERT software

The FILVERT code serves to compute the vertical velocity of advection  $v$  in  $n$  depth intervals  $z \in [h_k, H_k]$  ( $k=1, 2, \dots, n$ ) of the section under study on the basis of the measured  $T$ ,  $I$ , and  $A$  distribution with depth. The algorithm solves the one-dimensional steady-state equation for energy conservation, in Cartesian co-ordinates

$$dq/dz - A = 0, \quad (2)$$

where  $q$  is the energy flow density [Landau and Lifshits, 1986]. The parameter  $q$  consists of the conductive  $q_c$  and advective  $q_a$  constituents:

$$q(z) = q_c(z) + q_a(z), \quad (3)$$

where

$$q_c = -I \, dT/dz, \quad (1')$$

$$q_a = \mathbf{r} v h_w = \mathbf{r} v \int_T^c dT, \quad (4)$$

where  $\mathbf{r}$  and  $c$  are the density and specific heat capacity of water respectively,  $v$  is an "effective" vertical velocity of advection,  $h_w$  is the specific enthalpy of water,  $T$  is the Kelvin temperature.

The parameter  $v$  reflects the total contribution of the two main heat carriers – underground water and host rock – into the advective heat transfer. Let the water percolate at the velocity  $v_w$  through the host rock, whose density is  $\mathbf{r}_0$ , heat capacity is  $c_r$  (with allowance for its water saturation), and velocity (due to the tectonic movement) is  $v_0$ . In such conditions, the total contribution of the vertical fluid-rock advection into the energy balance in a co-ordinate system fixed at the Earth's surface, is

$$\begin{aligned} dq_a/dz &= \mathbf{r} v_w dh_w/dz + \mathbf{r}_0 v_0 dh_0/dz = \\ &= (c_r \mathbf{r} v_w + c_0 \mathbf{r}_0 v_0) dT/dz, \end{aligned} \quad (5)$$

where  $\mathbf{r} v_w$  and  $\mathbf{r}_0 v_0$  are the densities of fluid and rock mass fluxes respectively;  $h_0 = \int_T^{c_0} dT$  is the specific enthalpy of rock. Substituting  $q_a$  (4) into eq. (5) gives an expression for the effective velocity  $v$ :

$$v = v_w + v_0 (c_0 \mathbf{r}_0)/(c_r \mathbf{r}). \quad (6)$$

Such a representation of the effective velocity simplifies the calculation, since, in many cases (in the absence of phase transitions), the volume capacity of water  $c_r \mathbf{r}$  weakly varies with depth and may be set  $c_r \mathbf{r} = 1 \text{ cal}/(\text{cm}^3 \text{ K}) = 4.19 \times 10^6 \text{ J}/(\text{m}^3 \text{ K})$ .

The energy flow density  $q$  can vary with depth, owing to heat generation (take-up) by various sources (sinks). The most wide-spread heat sources are radioactive decay and exothermic reactions (rock hydration, oxidation, and others). Conversely, heat is absorbed in processes of rock transformation and the burial of organic matter at the early catagenesis stage (see the brief review by Sergienko [1996]). However, estimates

[e.g., Smyslov et al., 1979; Yakovlev, 1985] show that, on the background of the heat flow from the mantle, these exo- and endothermic processes make a subordinate contribution into the heat balance of layers of thickness of up to a few hundreds and thousands of meters. Furthermore, the conventional determinations of heat production  $A$  provide only a generalized picture of its vertical variations. For these reasons, the model in question was simplified:  $A$  was used as the constant in each of the design depth intervals; i.e., the step function

$$A_k = \text{const}, \quad z \in [h_k, H_k], \quad (k = 1, 2, \dots, n) \quad (7)$$

is used.

It is apparent that the one-dimensional model of the energy balance (2) does not consider any factors other than water-rock advection and heat generation which are able to complicate the conductive heat transfer (e.g., unsteady-state temperature distribution, lateral heat transfer, heat flux refraction, etc.). Such factors are not usually studied with suitable accuracy for this work, and introducing them into the model would not make it more realistic. Furthermore, in many cases, the fluid flow velocity is rather high (no less than a few mm/yr), and the influence of other factors on the thermal field is negligibly small, as already noted. Nevertheless, the possible effect of any factors, neglected in apparent form, should present in latent mode in the calculated velocity  $v$ , which is the only design (unknown) parameter of eq. (2).

We integrate (2) and obtain the equation for energy conservation in the form

$$-I \, dT/dz + c_r \mathbf{r} v T - Az = q^*, \quad (8)$$

where  $q^*$  is an arbitrary constant of integration. The constant  $q^*$  is so chosen that its physical meaning as well as expected value are close to those of the energy flow density ( $q - Az$ ) in an arbitrary point  $z = Z$ :  $q^* \approx q - Az$ , since  $h \approx cT$  (see comments in more detail below).

The procedure for calculating  $v$  and  $q^*$  is based on the mathematics, as follows. The design depth interval  $[Z_k, Z_{k+1}]$  is divided into several ( $J \geq 3$ ) integrating subintervals with the boundaries  $Z_j$  and  $Z_{j+1}$  ( $j = 1, 2, \dots, J$ ). Dividing all the terms in (8) by  $I$ , we integrate the obtained equation in each  $j$ th subinterval from  $Z_j$  to  $Z_{j+1}$  and, going to the finite differences ( $dz \rightarrow \Delta z$ ), get the  $J$  algebraic equations with two unknowns,  $v$  and  $q^*$ :

$$a_j v - b_j q^* - c_j = 0, \quad (j = 1, 2, \dots, J; J \geq 3), \quad (9)$$

where

$$a_j = c_r \Delta z / 2 \sum_j (T_j / I_j + T_{j+1} / I_{j+1}), \quad (10)$$

$$b_j = \Delta z / 2 \sum_j (1/I_j + 1/I_{j+1}), \quad (11)$$

$$c_j = \Delta T_j + A \Delta z / 2 \sum_j (z_j / I_j + z_{j+1} / I_{j+1}), \quad (12)$$

$\Delta T_j$  being the temperature drop between the bottom and top of the  $j$ th subinterval. The subscript  $i$  in (10)–(11) takes values  $i = 1, 2, \dots, I$ , where  $I \geq 5$  is the number of approximation steps in the  $j$ th interval.

The system of  $J \geq 3$  equations (9) for the two unknowns,  $v$  and  $q^*$ , is overdetermined. However, there exists a pair of optimum values,  $v = v_{\text{opt}}$  and  $q^* = q_{\text{opt}}^*$ , that approximately satisfy each of the equations:

$$a_j v_{\text{opt}} - b_j q_{\text{opt}}^* - c_j = \Delta \neq 0, \quad (j = 1, 2, \dots, J). \quad (13)$$

The solution  $(v_{\text{opt}}, q_{\text{opt}}^*)$  is optimal provided that the sum of squared residuals reaches its minimum:

$$D(v, q^*) = \sum_{j=1}^J \Delta_j^2 \rightarrow \min = D(v_{\text{opt}}, q_{\text{opt}}^*), \quad (14)$$

where  $D(v, q^*)$  is the total squared residual. This condition holds true, if

$$\partial D / \partial v = \partial D / \partial q^* = 0. \quad (15)$$

Substituting (14) into (15), we obtain the desired solution

$$\begin{aligned} v_{\text{opt}} &= \frac{\sum b_j^2 \sum a_j c_j - \sum a_j b_j \sum b_j c_j}{\sum a_j^2 \sum b_j^2 - (\sum a_j b_j)^2}, \\ q_{\text{opt}}^* &= \frac{\sum b_j c_j - v_{\text{opt}} \sum a_j b_j}{\sum b_j^2}. \end{aligned} \quad (16)$$

The design errors of computed  $v_{\text{opt}}$  and  $q_{\text{opt}}^*$  are

$$\begin{aligned} d_v &= \frac{\sum b_j^2 \sum a_j \Delta_j - \sum a_j b_j \sum b_j \Delta_j}{v - r \left( (\sum a_j b_j)^2 - \sum a_j^2 \sum b_j^2 \right)}, \\ d_q &= \frac{\sum a_j b_j \sum a_j \Delta_j - \sum a_j^2 \sum b_j \Delta_j}{q \left( (\sum a_j b_j)^2 - \sum a_j^2 \sum b_j^2 \right)}. \end{aligned} \quad (17)$$

where  $\Delta_j$  is the model net error. It includes the errors of measuring the input parameters and of approximating the functions by finite decrements. The design errors  $d_v$  and  $d_q$  depend mainly on the accuracy of measuring the input data,  $T$ ,  $I$ , and  $A$ . Analysis shows that the difference procedure realized in this work fits the necessary condition of convergence and conditional stability. The stability range is bounded by the minimal absolute values of the required parameters  $|v| \geq \sim n \cdot (0.01-0.1)$  mm/yr and  $|q^*| \geq \sim 1-10$  mW/m<sup>2</sup> (on the order of magnitude). These bounds lie below the usual natural values and are confirmed by FILVERT numerical experiments on test data and the above-mentioned natural data.

The FILVERT algorithm is performed in two FORTRAN-90 versions. The first of these requires a preliminary division of the measured geothermal section into design intervals taking into account the geological structure of the section under study. The optimum solution is sought in each interval by sequential tests of all possible subdivisions of the interval into integration subintervals, so that the number of these subintervals  $J$  runs values increasing from  $J_0 = 3$  to  $J_{\text{max}}$ . Correspondingly, the number of approximation steps  $I$  decreases from  $I_0$  to  $I_{\text{min}} = 5$ . The values  $v$ ,  $q^*$ , and  $D$  are computed for each of the subdivisions. Finally, the program finds and prints the pair values  $(v_{\text{opt}}, q_{\text{opt}}^*)$ , the design errors  $d_v$  and  $d_q$ , and the related value of total squared residual  $D = D_{\text{min}}$  for the best subdivision of each design interval.

The choice of the boundaries of design intervals is essentially subjective, and an accurate solution requires the testing of other possible positions of the boundaries. This routine is automated in the second version of FILVERT, by sampling (scanning) the vicinity of the top and bottom of the chosen intervals at a given step in depth. The scanning procedure greatly improves the accuracy of the final solution.

The output data are used to construct the diagrams of the velocity  $v$  vertical distribution. Fig. 2 demonstrates an example of such a diagram reflecting structure and kinematics of fluid fluxes in the studied section (see a discussion below).

### 2.3 Evaluating the deep heat flow density

The second main sought-for parameter, deep heat flow density  $q_0$ , is estimated with the help of a plot constructed on coordinates  $(v, q^*)$  (Fig. 3). Exploration of actual holes showed that the set of pair solutions found forms a close cloud of points, which can be approximated by the straight line

$$q^* = B v + q_0^*, \quad (18)$$

where  $B$  and  $q_0^*$  are empirical constants. They likely depend on the local tectonic structure and geothermal conditions in the drilled fragment of lithosphere.

As stated above, the constant of integration  $q^*$  approximately equals to the energy flow density  $q - Az$  at each arbitrary point  $z = Z$ :

$$q^* = -I dT/dz + r v(cT) - Az \approx q_c + q_a - Az = q - Az \quad (19)$$

(as  $cT \approx h$ ). Naturally, the contribution of heat generation  $Az$  to the total energy flow is negligible in depth intervals of a few kilometers from the Earth's surface. Therefore, the FILVERT code yields for each of such intervals

$$q^*(z) \approx q(z). \quad (20)$$

It is apparent that the approximate eq. (20) remains valid, if the advective constituent of heat flux is zero, i.e.  $v = 0$ . In this case of pure conductive heat transfer one can state that

$$q^*|_{v=0} = q_0^* \approx q_c = q_0. \quad (21)$$

Thus, the  $q^*$ -intercept, for  $v = 0$ , of the line (18) at the plot (Fig. 3) may be considered to be close to the deep heat flow density  $q_0$  (at the assumption of pure conductive heat transfer in deep strata). The accuracy of evaluating the  $q_0$ -value,  $|d|_{\text{av}}$ , is found as the average error in the calculated  $v$  and  $q^*$ :

$$q_0 \approx q_0^* (1 \pm |d|_{\text{av}}), \quad (22)$$

## 3. AN EXAMPLE OF RESULTS AND DISCUSSION

Figure 2 shows the vertical variations of the velocity  $v$ , calculated using the FILVERT code for different intervals in the Saatly super deep hole, Azerbaijan, illustrating the structure and the kinematics of fluid fluxes [Yakovlev, 1999]. The rectangles show the  $v$ -values ranging in each depth interval within design error. The drilled section consists of the Cenozoic

molassa (interval 0-2.8 km), Upper-Cretaceous limestones (2.8-3.5 km), and Jurassic-Cretaceous volcanics (mainly basalts) subjected to greenschist metamorphism (3.5-8.3 km). A hydrodynamic inversion is revealed here: near-lithostatic fluid pressures (piezomaximum), observed in the central part of the molassa section (depth of 1.5-1.6 km), decrease with depth down to near-hydrostatic values in lower zones of the volcanic section [Borevsky et al., 1995; Yakovlev, 1999]. This inversion is due to catagenesis of sediments and squeezing of the elision fluids from the molassa, with consequent water absorption by volcanics subjected to metamorphic hydration. That is why a downward fluid flow occurs below the depth of 1.6 km having the moderate velocity of 1 mm/yr, as is seen from the diagram (Fig. 2), whereas above this depth, fluids move upward at the velocity of  $-2$  mm/yr. On the integral background of downward flux, cellular fluid currents of various (positive and even negative) velocities may be seen within local intervals, where the percolating water is accumulated because of enhanced permeability of host rocks.

The  $v - q$  plot (Fig. 3) represents the full set of pair  $(v, q^*)$  solutions obtained at the Saatly hole. The narrow cloud of figurative points is approximated by straight regression line

$$q^* = 44.34v - 29.54. \quad (23)$$

This line is almost of functional meaning (the correlation coefficient is 0.999) despite the high design errors in individual  $v$ - $q$ -values ( $d_{av.} = 0.5$ ). Equation (23) provides the deep heat flow density  $q_0 \approx q^*_0 = 30 \pm 15$  mW/m<sup>2</sup> at the Saatly drilling site. This result agrees well with the estimation of the heat flow density on the mantle surface,  $q_0 = 24.7$  mW/m<sup>2</sup> [Smirnov, 1980].

#### 4. CONCLUSION

The software proposed to study structure and kinematics of fluid fluxes (vertical variations of the advection velocity) in the borehole section and to determine deep heat flow density at the drilling site uses only thermal data (hydrogeological information need not be invoked). The algorithm takes into account all regular and random variations in the original parameters (temperature  $T$ , heat conductivity  $I$ , and heat production  $A$ ). As initial information, one can use data either from an individual hole or from a set of holes outcropping the geological section where the thermal field is variably distorted by fluid advection.

The algorithm processes convergence and the conditional stability. It gives reliable results both for  $v(z)$  and  $q_0$ , if the calculated velocity  $v(z)$  at depths considered is no less than tenths of 1 mm/yr and the coupled energy flux density  $q(z)$  (which includes conductive and advective constituents) is no less than 10 mW/m<sup>2</sup>.

#### ACKNOWLEDGEMENTS

This study was sponsored by the Russian Foundation for Basic Research (grant no. 99-05-64800). The author is grateful to V.N. Prupis (USA) for his valuable advice in developing the

algorithm, L.V. Borevsky (Russia) and L. Lenkey (Hungary) for their assistance in setting up the numerical experiments on natural objects, and to Russian colleagues A.O. Gliko, B.G. Polyak, V.P. Pimenov, and V.B. Gubin for the consultations.

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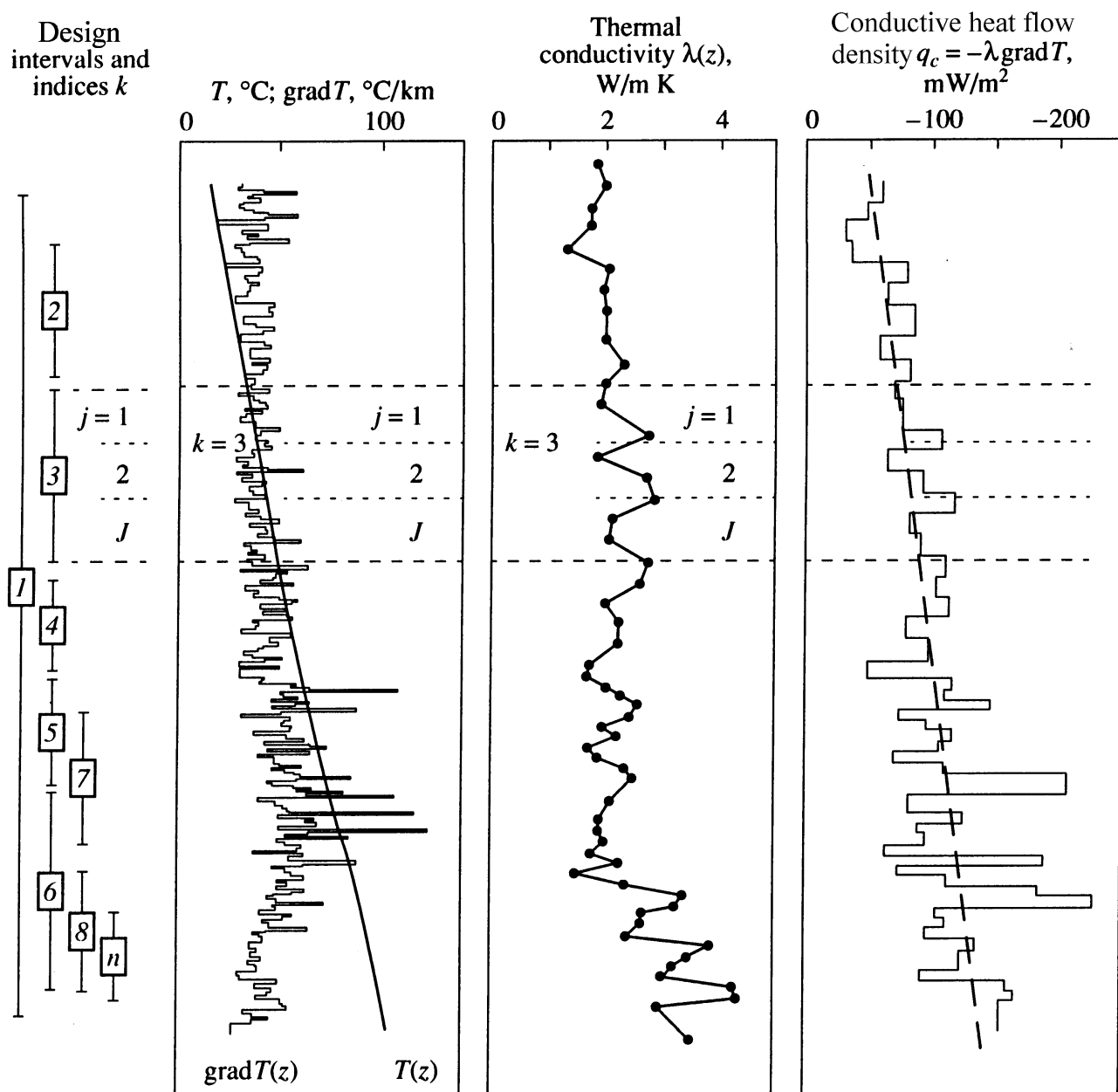


Figure 1. General view of the original geothermal data used in the FILVERT computer code. An example of the division of the section in question into  $n$  design intervals (numbered by the subscript  $k$ ) and  $J$  integration subintervals (subscript  $j$ ) is shown on the left.

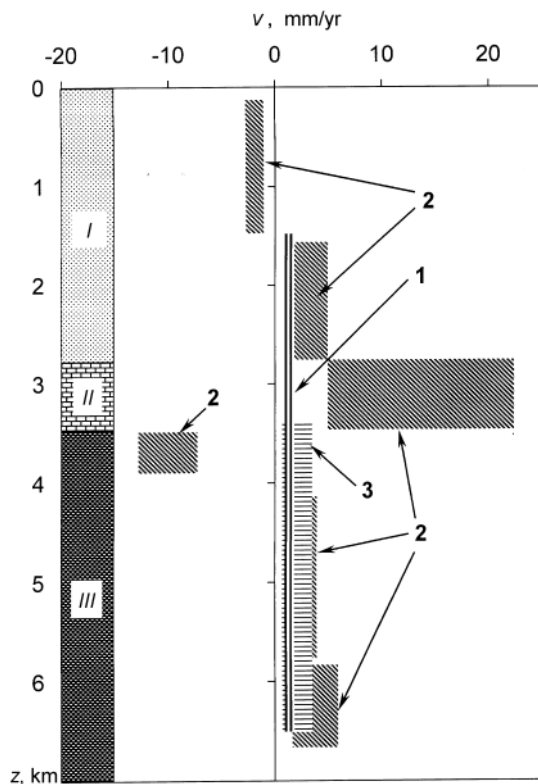


Figure 2. Variations of the effective velocity of advection  $v$  in the Saatly hole section, computed by means of the FILVERT code (Yakovlev, 1999). *I-III* – lithological units in the section: *I* – Cenozoic molassa, *II* – Upper-Cretaceous limestones, *III* – Jurassic-Cretaceous volcanics; *1-3* – ranges of the velocity  $v$  calculated at design errors  $d_v$  within various depth intervals: *1* – within the depths below the level of piezomaximum observed in the central part of the molassa sequence (1.5-1.6 km), *2* – in local depth intervals, *3* – within the volcanic sequence as a whole.

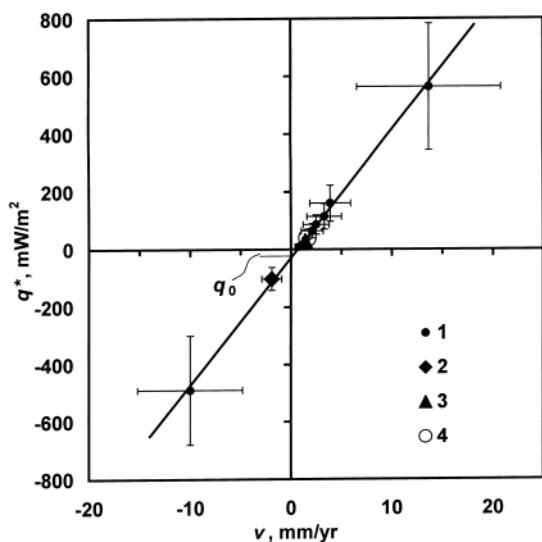


Figure 3. Diagram of the graphic-analytical processing of a set of pair solutions  $(v_{\text{opt}}, q^*_{\text{opt}})_k$ , obtained by means of the FILVERT code using thermal data from the Saatly hole (Yakovlev, 1999), with the purpose of determining the deep heat flow density  $q_0$ . *1-4* – figurative points characterizing the pair solutions: *1* – within local depth intervals, *2* – above the piezomaximum zone (depth < 1.5 km), *3* – below the piezomaximum zone (depth > 1.6 km), *4* – within the studied section as a whole. The set of solutions is approximated by regression line  $q = 44.34 v - 29.54$  (correlation coefficient  $r^2 = 0.9984$ ), where the dimensionalities are:  $q = [\text{mW}/\text{m}^2]$ ,  $v = [\text{mm}/\text{yr}]$ . The heat flow density at the Saatly drilling site is estimated as  $q_0 = 30 \pm 15 \text{ mW}/\text{m}^2$ .